wwPDB NMR Structure Validation Summary Report (i)

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PDB ID	:	1OCI
Title	:	[3.2.0]bcANA:DNA
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This is a wwPDB NMR Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	FAILED
Mogul	:	1.8.4, CSD as541be (2020)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

There are no overall percentile quality scores available for this entry.

The sequence quality summary graphics cannot be shown.

2 Ensemble composition and analysis (i)

This entry contains 40 models. This entry does not contain polypeptide chains, therefore identification of well-defined residues and clustering analysis are not possible. All residues are included in the validation scores.

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 572 atoms, of which 207 are hydrogens and 0 are deuteriums.

- Molecule 1 is a DNA chain called 5'-D(*CP*TP*GP*A TLBP*AP*TP*GP*CP)-3'.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
1	A	9	287	89	104	32	54	8	0

- Molecule 2 is a DNA chain called 5'-D(*GP*CP*AP*TP*AP*TP*CP*AP*GP)-3'.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
2	B	9	285	88	103	35	51	8	0

4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: 5'-D(*CP*TP*GP*A TLBP*AP*TP*GP*CP)-3'

Chain A: 89% 11%

• Molecule 2: 5'-D(*GP*CP*AP*TP*AP*TP*CP*AP*GP)-3'

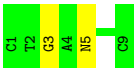
Chain B: 89% 11%

4.2 Residue scores for the representative (author defined) model from the NMR ensemble

The representative model is number 6. Colouring as in section 4.1 above.

• Molecule 1: 5'-D(*CP*TP*GP*A TLBP*AP*TP*GP*CP)-3'

Chain A: 78% 22%



• Molecule 2: 5'-D(*GP*CP*AP*TP*AP*TP*CP*AP*GP)-3'

Chain B: 89% 11%

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *simulated annealing*.

Of the 40 calculated structures, 40 were deposited, based on the following criterion: *?*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
Amber	refinement	
MARDIGRAS	structure solution	
Amber	structure solution	

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

MolProbity failed to run properly - this section will have to be empty.

6.2 Too-close contacts (i)

MolProbity failed to run properly - this section will have to be empty.

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

MolProbity failed to run properly - this section will have to be empty.

6.3.2 Protein sidechains (i)

MolProbity failed to run properly - this section will have to be empty.

6.3.3 RNA (i)

MolProbity failed to run properly - this section will have to be empty.

6.4 Non-standard residues in protein, DNA, RNA chains (i)

MolProbity failed to run properly - this section will have to be empty.

6.5 Carbohydrates (i)

MolProbity failed to run properly - this section will have to be empty.

6.6 Ligand geometry (i)

MolProbity failed to run properly - this section will have to be empty.

6.7 Other polymers (i)

MolProbity failed to run properly - this section will have to be empty.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

No chemical shift data were provided